d01 - Quadrature d01xbc

# **NAG C Library Function Document**

# nag multid quad monte carlo 1 (d01xbc)

## 1 Purpose

nag\_multid\_quad\_monte\_carlo\_1 (d01xbc) evaluates an approximation to the integral of a function over a hyper-rectangular region, using a Monte Carlo method. An approximate relative error estimate is also returned. This routine is suitable for low accuracy work.

## 2 Specification

## 3 Description

This function uses an adaptive Monte Carlo method based on the algorithm described by Lautrup (1971). It is implemented for integrals of the form:

$$\int_{a_1}^{b_1} \int_{a_2}^{b_2} \dots \int_{a_n}^{b_n} f(x_1, x_2, \dots, x_n) \ dx_n \dots dx_2 dx_1.$$

Upon entry, unless the parameter **method** has the value **Nag\_OneIteration**, the routine subdivides the integration region into a number of equal volume subregions. Inside each subregion the integral and the variance are estimated by means of pseudo-random sampling. All contributions are added together to produce an estimate for the whole integral and total variance. The variance along each co-ordinate axis is determined and the routine uses this information to increase the density and change the widths of the sub-intervals along each axis, so as to reduce the total variance. The total number of subregions is then increased by a factor of two and the program recycles for another iteration. The program stops when a desired accuracy has been reached or too many integral evaluations are needed for the next cycle.

## 4 Parameters

1: **ndim** – Integer Input

On entry: the number of dimensions of the integral, n.

Constraint:  $\mathbf{ndim} \geq 1$ .

2:  $\mathbf{f}$  – function supplied by user

Function

The function f, supplied by the user, must return the value of the integrand f at a given point. The specification of f is:

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2: x[ndim] - double

Input

On entry: the co-ordinates of the point at which the integrand must be evaluated.

3: **comm** – Nag User \*

On entry/on exit: pointer to a structure of type Nag User with the following member:

**p** – Pointer Input/Output

On entry/on exit: the pointer **comm**→**p** should be cast to the required type, e.g., struct user \*s = (struct user \*)comm->p, to obtain the original object's address with appropriate type. (See the argument **comm** below.)

3: **method** – Nag MCMethod

Input

On entry: the method to be used.

If **method** = **Nag\_OneIteration**, then the function uses only one iteration of a crude Monte Carlo method with **maxcls** sample points.

If **method** = **Nag\_ManyIterations**, then the function subdivides the integration region into a number of equal volume subregions.

Constraint: method = Nag\_OneIteration or Nag\_ManyIterations.

4: **cont** – Nag Start

Input

On entry: the continuation state of the evaluation of the integrand.

If **cont** = **Nag\_Cold**, indicates that this is the first call to the function with the current integrand and parameters **ndim**, **a** and **b**.

If **cont** = **Nag\_Hot**, indicates that a previous call has been made with the same parameters **ndim**, **a** and **b** with the same integrand. Please note that **method** must not be changed.

If **cont** = **Nag\_Warm**, indicates that a previous call has been made with the same parameters **ndim**, **a** and **b** but that the integrand is new. Please note that **method** must not be changed.

Constraint: cont = Nag Cold, Nag Warm or Nag Hot.

5: **a[ndim]** – double

Input

On entry: the lower limits of integration,  $a_i$ , for i = 1, 2, ..., n.

6: **b[ndim]** – double

Input

On entry: the upper limits of integration,  $b_i$ , for i = 1, 2, ..., n.

7: **mincls** – Integer \*

Input/Output

On entry: mincls must be set to the minimum number of integrand evaluations to be allowed.

Constraint:  $0 \le \text{mincls} < \text{maxcls}$ .

On exit: mincls contains the total number of integrand evaluations actually used by nag\_multid\_quad\_monte\_carlo\_1.

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8: **maxcls** – Integer

Input

On entry: the maximum number of integrand evaluations to be allowed. In the continuation case this is the number of new integrand evaluations to be allowed. These counts do not include zero integrand values.

Constraints:

maxcls > mincls;

 $maxcls \ge 4 \times (ndim + 1)$ .

9: **eps** – double

Input

On entry: the relative accuracy required.

Constraint: eps > 0.0.

10: **finest** – double \*

Output

On exit: the best estimate obtained for the integral.

11: **acc** – double \*

Output

On exit: the estimated relative accuracy of finest.

12: **comm arr** – double \*\*

Input/Output

On entry: if **cont** = **Nag\_Warm** or **Nag\_Hot**, the memory pointed to and allocated by a previous call of nag multid quad monte carlo\_1 must be unchanged.

If  $cont = Nag\_Cold$  then appropriate memory is allocated internally by nag\\_multid\_quad\_monte\_carlo\_1.

On exit: **comm\_arr** contains information about the current sub-interval structure which could be used in later calls of nag\_multid\_quad\_monte\_carlo\_1. In particular, **comm\_arr**[j-1] gives the number of sub-intervals used along the jth co-ordinate axis.

When this information is no longer useful, or before a subsequent call to nag\_multid\_quad\_monte\_carlo\_1 with **cont** = **Nag\_Cold** is made, the user should free the storage contained in this pointer using the NAG macro **NAG\_FREE**. Note this memory will have been allocated and needs to be freed only if the error exit **NE\_NOERROR** or **NE\_QUAD\_MAX\_INTEGRAND\_EVAL** occurs. Otherwise, no memory needs to be freed.

13: **comm** – Nag\_User \*

On entry/on exit: pointer to a structure of type Nag User with the following member:

**p** – Pointer Input/Output

On entry/on exit: the pointer p, of type Pointer, allows the user to communicate information to and from the user-defined function f(). An object of the required type should be declared by the user, e.g., a structure, and its address assigned to the pointer p by means of a cast to Pointer in the calling program, e.g., comm.p = (Pointer)&s. The type Pointer is void \*.

14: **fail** – NagError \*

Input/Output

The NAG error parameter (see the Essential Introduction).

Users are recommended to declare and initialise fail and set fail.print = TRUE for this function.

## 5 Error Indicators and Warnings

#### NE INT ARG LE

On entry, **mincls** must not be less than or equal to 0: **mincls** =  $\langle value \rangle$ .

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#### NE INT ARG LT

On entry, **ndim** must not be less than 1: **ndim** =  $\langle value \rangle$ .

### NE REAL ARG LT

On entry, eps must not be less than 0.0: eps =  $\langle value \rangle$ .

#### NE 2 INT ARG GE

On entry, **mincls** =  $\langle value \rangle$  while **maxcls** =  $\langle value \rangle$ . These parameters must satisfy **mincls**  $\langle$  **maxcls**.

#### NE 2 INT ARG LT

On entry, **maxcls** =  $\langle value \rangle$  while **ndim** =  $\langle value \rangle$ . These parameters must satisfy **maxcls**  $\geq 4 \times (ndim+1)$ .

### **NE BAD PARAM**

On entry, parameter **method** had an illegal value. On entry, parameter **cont** had an illegal value.

### NE QUAD MAX INTEGRAND EVAL

maxcls was too small to obtain the required accuracy.

In this case nag\_multid\_quad\_monte\_carlo\_1 returns a value of **finest** with estimated relative error **acc**, but **acc** will be greater than **eps**. This error exit may be taken before **maxcls** non-zero integrand evaluations have actually occurred, if the routine calculates that the current estimates could not be improved before **maxcls** was exceeded.

### NE\_ALLOC\_FAIL

Memory allocation failed.

#### **6** Further Comments

The running time for nag\_multid\_quad\_monte\_carlo\_1 will usually be dominated by the time used to evaluate the integrand **f**, so the maximum time that could be used is approximately proportional to **maxcls**.

For some integrands, particularly those that are poorly behaved in a small part of the integration region, this function may terminate with a value of **acc** which is significantly smaller than the actual relative error. This should be suspected if the returned value of **mincls** is small relative to the expected difficulty of the integral. Where this occurs, nag\_multid\_quad\_monte\_carlo\_1 should be called again, but with a higher entry value of **mincls** (e.g., twice the returned value) and the results compared with those from the previous call.

The exact values of **finest** and **acc** on return will depend (within statistical limits) on the sequence of random numbers generated within this function by calls to nag\_random\_continuous\_uniform (g05cac). Separate runs will produce identical answers unless the part of the program executed prior to calling this function also calls (directly or indirectly) routines from Chapter g05, and the series of such calls differs between runs. If desired, the user may ensure the identity or difference between runs of the results returned by this function, by calling nag\_random\_init\_repeatable (g05cbc) or nag\_random\_init\_nonrepeatable (g05ccc) respectively, immediately before calling this function.

## 6.1 Accuracy

A relative error estimate is output through the parameter **acc**. The confidence factor is set so that the actual error should be less than **acc** 90% of the time. If a user desires a higher confidence level then a smaller value of **eps** should be used.

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#### 6.2 References

Lautrup B (1971) An adaptive multi-dimensional integration procedure *Proc. 2nd Coll. Advanced Methods in Theoretical Physics, Marseille* 

### 7 See Also

nag multid quad adapt 1 (d01wcc)

## 8 Example

This example program calculates the integral

$$\int_0^1 \int_0^1 \int_0^1 \int_0^1 \frac{4x_1 x_3^2 \exp(2x_1 x_3)}{(1 + x_2 + x_4)^2} dx_1 dx_2 dx_3 dx_4 = 0.575364.$$

### 8.1 Program Text

```
/* nag_multid_quad_monte_carlo_1(d01xbc) Example Program
 * Copyright 1998 Numerical Algorithms Group.
 * Mark 5, 1998.
 * Mark 6 revised, 2000.
#include <nag.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <math.h>
#include <nagd01.h>
static double f(Integer ndim, double x[], Nag_User *comm);
#define NDIM 4
#define MAXCLS 20000
main()
  double a[4], b[4];
  Integer k, mincls;
  double finest;
  double acc, eps;
  Integer ndim = NDIM;
  Integer maxcls = MAXCLS;
  static NagError fail;
  double *comm_arr = (double *)0;
  Nag_MCMethod method;
  Nag_Start cont;
  Nag_User comm;
  Vprintf("d01xbc Example Program Results\n");
  for (k=0; k<4; ++k)
    {
      a[k] = 0.0;
      b[k] = 1.0;
```

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```
eps = 0.01;
 mincls = 1000;
 method = Nag_ManyIterations;
 cont = Nag_Cold;
 d01xbc(ndim, f, method, cont, a, b, &mincls, maxcls, eps,
        &finest, &acc, &comm_arr, &comm, &fail);
 if (fail.code != NE_NOERROR)
   Vprintf("%s\n", fail.message);
  if (fail.code == NE_NOERROR || fail.code == NE_QUAD_MAX_INTEGRAND_EVAL)
     Vprintf("Requested accuracy = %10.2e\n",eps);
     Vprintf("Estimated value = %10.5f\n", finest);
     Vprintf("Estimated accuracy = %10.2e\n", acc);
     Vprintf("Number of evaluations = %5ld\n", mincls);
     /* Free memory allocated internally */
     NAG_FREE(comm_arr);
     exit(EXIT_SUCCESS);
    }
 else
   exit(EXIT_FAILURE);
static double f(Integer ndim, double x[], Nag_User *comm)
 return x[0]*4.0*(x[2]*x[2])*exp(x[0]*2.0*x[2])/
    ((x[1]+1.0+x[3])*(x[1]+1.0+x[3]));
```

### 8.2 Program Data

None.

#### 8.3 Program Results

```
d01xbc Example Program Results
Requested accuracy = 1.00e-02
Estimated value = 0.57554
Estimated accuracy = 8.20e-03
Number of evaluations = 1728
```

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